

COMP

Emilio Esposito, Scott Wildman

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514 - Entropy-driven chemisorption of NO_x on phosphotungstic acid

Lennart Joos¹, lennart.joos@ugent.be, Steven Heylen², Tatjana Parac-Vogt³, Veronique Van Speybroeck¹, Christine E.A. Kirschhock², Johan A. Martens². (1) Center for Molecular Modeling, Ghent University, Ghent, Belgium, (2) Centre for Surface Chemistry and Catalysis, KU Leuven, Leuven, Belgium, (3) Molecular Design and Synthesis, KU Leuven, Leuven, Belgium

Nitrogen oxides (NO_x) -mostly caused by the combustion of fossil fuels- contribute to the formation of ozon, smog and acid rain, so lowering NO_x emissions to the atmosphere is desired. [1] Phosphotungstic acid is a selective NO_x adsorbent with high adsorption capacity that could be used to capture NO_x molecules from exhaust gases and later release them for processing. [2]

A variety of experimental and computational approaches - including ex-situ and in-situ X-ray diffraction, neutron diffraction, NMR and DFT calculations - determined the nature of the chemisorbed NO_x species and elucidated the reaction behavior.

Experiments show that at high temperature, NO_x adsorption occurs, while at low temperature, the reverse reaction takes place. DFT calculations could assign this behavior to the entropy change during the reaction. Upon chemisorption of 3 NO molecules and 3 NO₂ molecules, 15 water molecules are released from the phosphotungstic acid hexahydrate (See Figure). This gives rise to a positive reaction entropy whereas the reaction energy is also positive. The free energy is negative -and thus chemisorption occurs- when the temperature are sufficiently high.

The insights from this study will allow optimization of the adsorbent material for application in after-treatment systems for NO_x elimination.

□

[1] TEDxGhent talk: <http://youtu.be/SvhLtiBDJ3s>

[2] Heylen, S., Joos, L., Parac-Vogt, T. N., Van Speybroeck, V., Kirschhock, C. E. A. and Martens, J. A., *Angew. Chem. Int. Ed.* **2012**, 51 (44), 11010-11013

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